Ionization of Atomic Hydrogen in Strong Infrared Laser Fields

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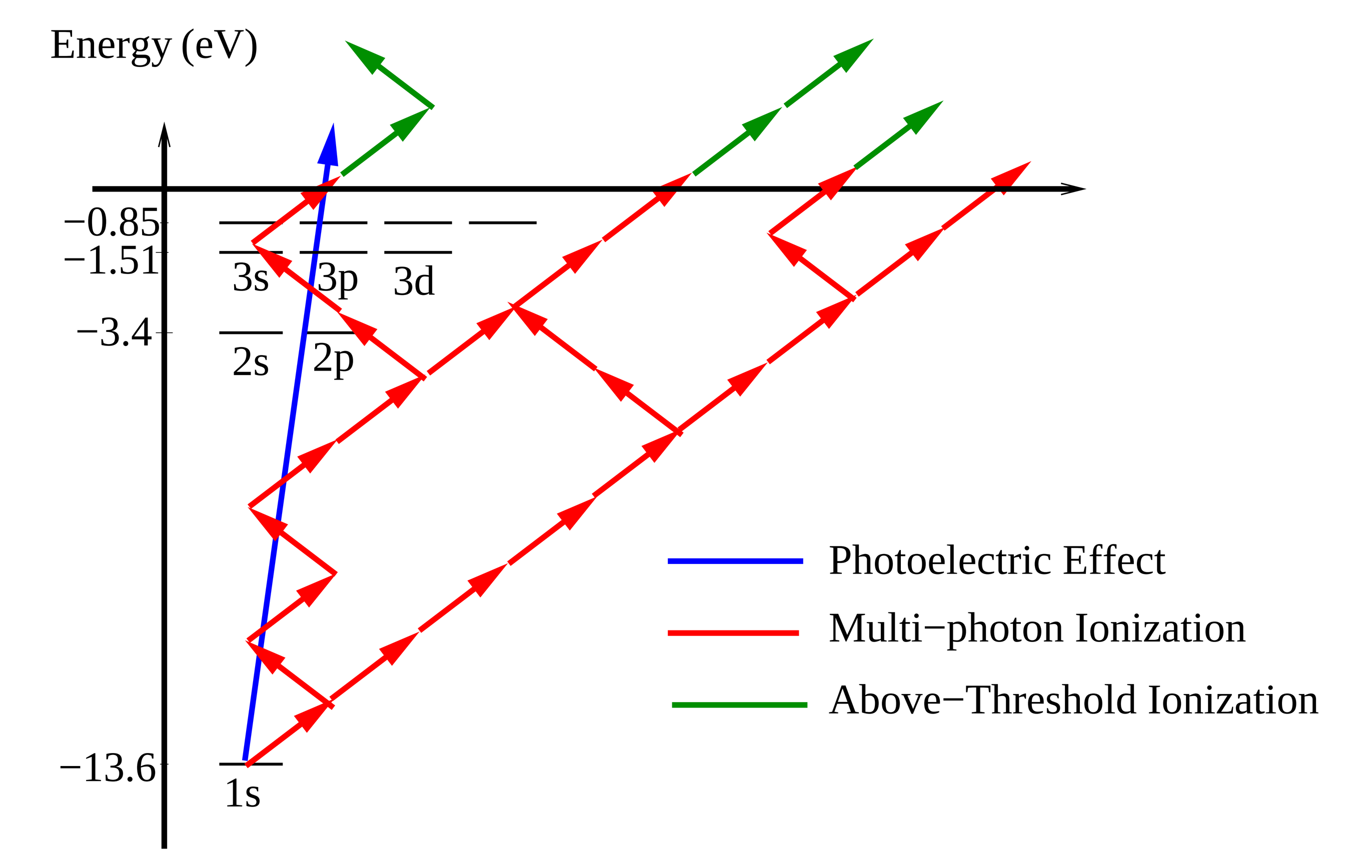
Abstract

We have used the matrix iteration method of Nurhuda and Faisal (Phys. Rev. A **60** (1999) 3125) to treat ionization of atomic hydrogen by a strong laser pulse. After testing our predictions against a variety of previous calculations, we present ejected-electron spectra as well as angular distributions for few-cycle infrared laser pulses with peak intensities of up to 10^{15} W/cm^2. The convergence of the results with the number of partial waves is a serious issue, which can be managed in a satisfactory way by using the velocity form of the electric dipole operator in connection with an efficient time-propagation scheme.

Introduction

- **1 attosecond** is one-millionth of one millionth of one millionth (10^{-18}) of a second.
- There are twice as many attoseconds in 1 second than seconds in the **age of the universe** (15 billion years)!
- The period for the $n = 1$ orbit in atomic hydrogen is about 150 attoseconds.
- Attosecond laser pulses provide a window to study the details of (valence) electron interactions in atoms and molecules.
- A major role for **theory** in attosecond science is to **suggest novel ways of investigating and controlling electronic processes** in matter on ultra-short time scales.
- Typical laser intensities in this field range from 10^{12} to 10^{15} W/cm^2.
- **10^{14} W/cm^2 is a million billion times stronger than the radiation that the Earth receives from the Sun directly above us on a clear day.**
- Such intensities can rip electrons away from atoms in very different ways from the **standard photoeffect**:
  - **Multi-photon ionization**
  - **Above-threshold ionization**
  - **Field (tunnel) ionization**

Single vs. Multi−Photon Ionization in Atomic Hydrogen



Numerical Method

- We start with the **Time-Dependent Schrödinger Equation**

$$\hat{\boldsymbol{H}}\Psi = i\frac{\partial}{\partial t}\Psi \qquad (1)$$

- In the **Length Form** of the electric dipole operator,

$$\hat{\boldsymbol{H}} = -\frac{1}{2}\nabla^2 + \frac{l(l+1)}{2r^2} - \frac{1}{r} + r\cos(\vartheta)\boldsymbol{E}(t) \qquad (2)$$

- In the **Velocity Form**, we have instead

$$\hat{\boldsymbol{H}} = -\frac{1}{2}\nabla^2 + \frac{l(l+1)}{2r^2} - \frac{1}{r} - \frac{i\boldsymbol{A}(t)}{c}\cdot\boldsymbol{\nabla} \qquad (3)$$

- We propagate the initial wavefunction $\Psi(\boldsymbol{r}, t = 0)$ in time using **Finite Differences**.
- In the **Crank-Nicholson Approximation**

$$\Psi(\boldsymbol{r}, t + \Delta t) \approx \frac{1 - i\hat{\boldsymbol{H}}\Delta t/2}{1 + i\hat{\boldsymbol{H}}\Delta t/2}\Psi(\boldsymbol{r}, t) \qquad (4)$$

it is difficult to calculate the "denominator", i.e., the inverse of a matrix at every time step.

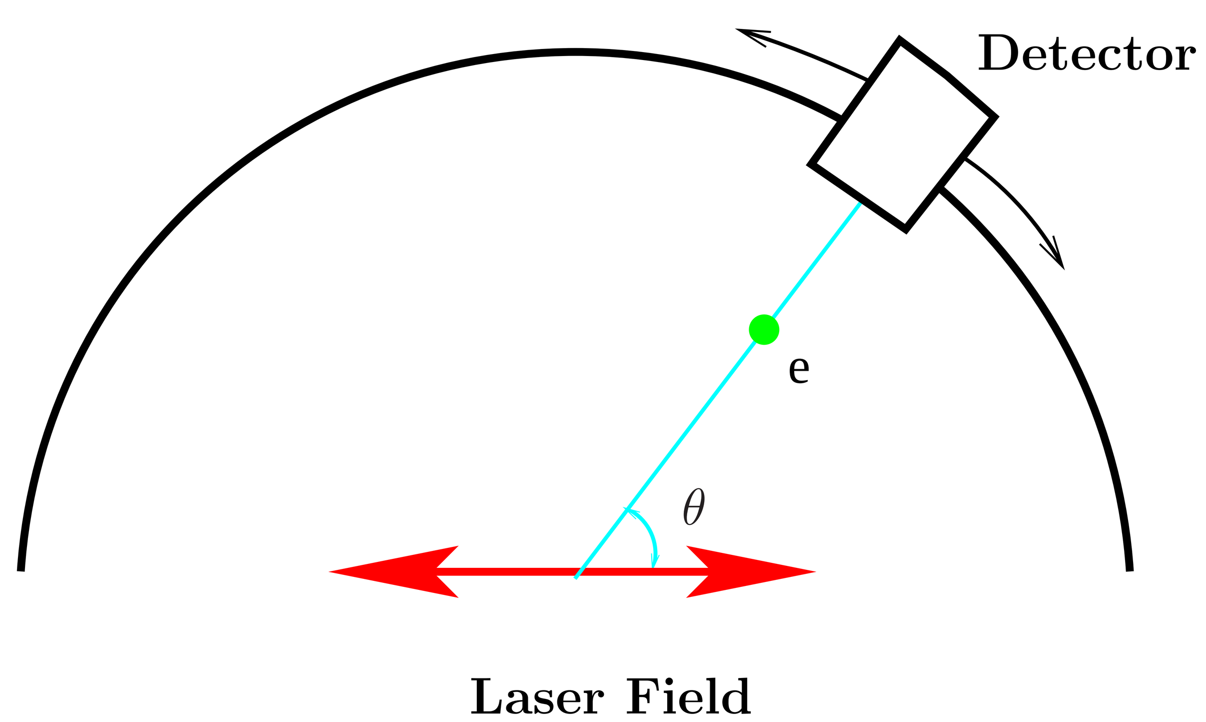
Matrix Iteration Method

- We define $1 + i\hat{\boldsymbol{H}}\Delta t/2 \equiv \hat{\boldsymbol{O}}_{\boldsymbol{D}} + \hat{\boldsymbol{O}}_{\boldsymbol{ND}}$
- and write $(1 + i\hat{\boldsymbol{H}}\Delta t/2)^{-1} \approx \boldsymbol{(1 - \hat{O}_D^{-1}\hat{O}_{ND} + \hat{O}_D^{-1}\hat{O}_{ND}\hat{O}_D^{-1}\hat{O}_{ND} + \ldots)\hat{O}_D^{-1}}$
- Taking 3−8 terms in the series expansion generally yields converged results.

Observables of Interest

- Observables are the **physical values** obtained from $\Psi(\boldsymbol{r}, t \to \infty)$ in a **measurement**.

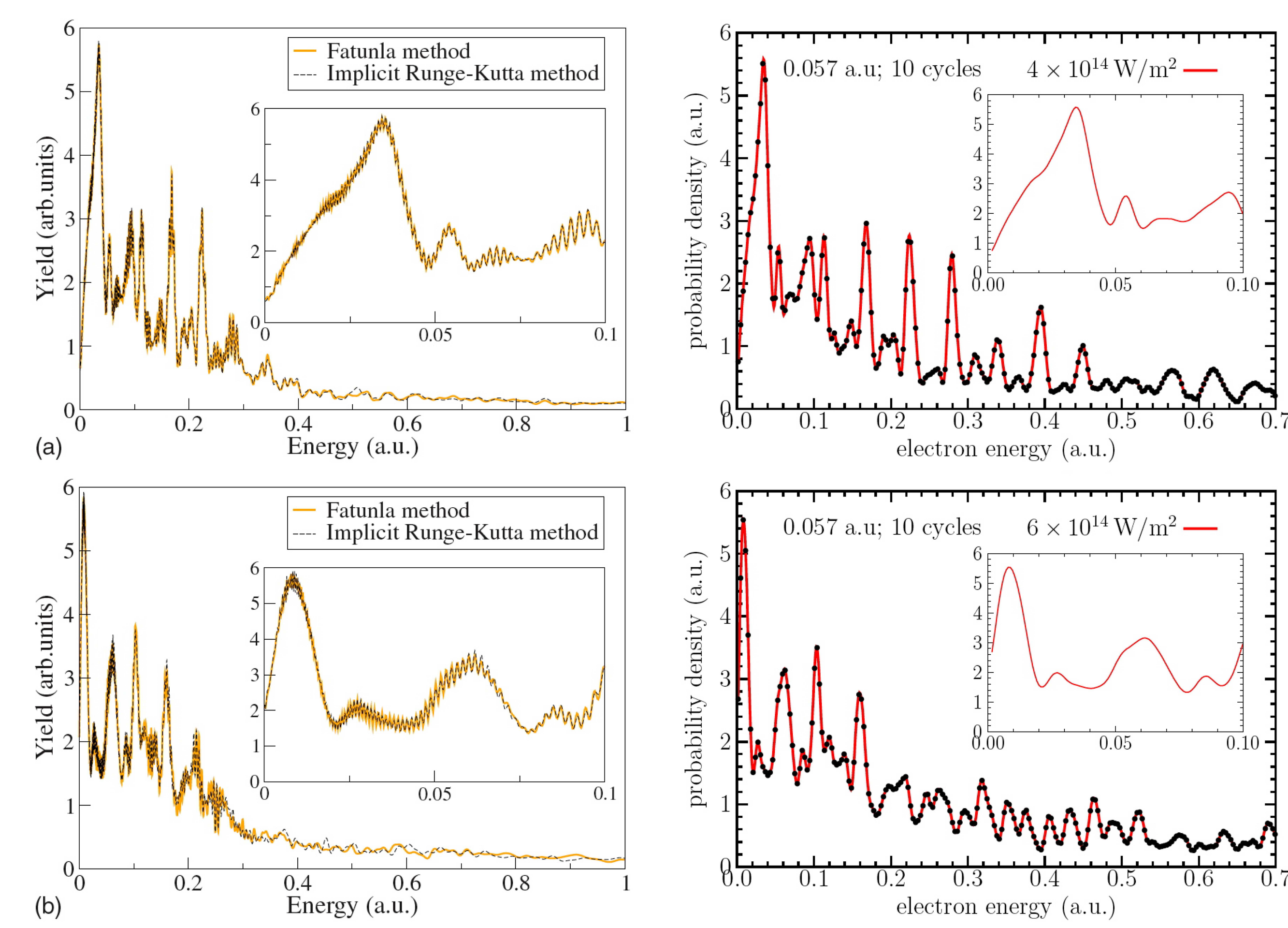
Scheme of an Angular-Distribution Experiment



- **Photoelectron spectrum**: How many electrons come out, and with what energies?
- **Angular distribution of photoelectrons**: Where do the electrons go?

Results

Madroñero and Piraux (2009) | **Our Calculation (2010, in press)**



- The recent calculations by Madroñero and Piraux (Phys. Rev. A **80** (2009), 033409) exhibit two serious problems:
  - **unphysical oscillations**, most likely due to the insufficient size of their numerical grid;
  - **lack of convergence** for energies above ≈ 0.3 a.u., due to a limited number of basis functions.
- We pushed our calculations to even **higher intensities** (10^{15} W/cm^2) **and energies** up to 4 a.u.
- **Measurements are currently in progress** at Griffith University in Brisbane (Australia).
- **We generated movies to illustrate the time dependence of the ionization process.**
- Below are snapshots for a 4-cycle pulse with a $\sin^2$ envelope function, a maximum intensity of 10^{15} W/cm^2, and a central wavelength of 152 nm.